Computational Accelerator Physics

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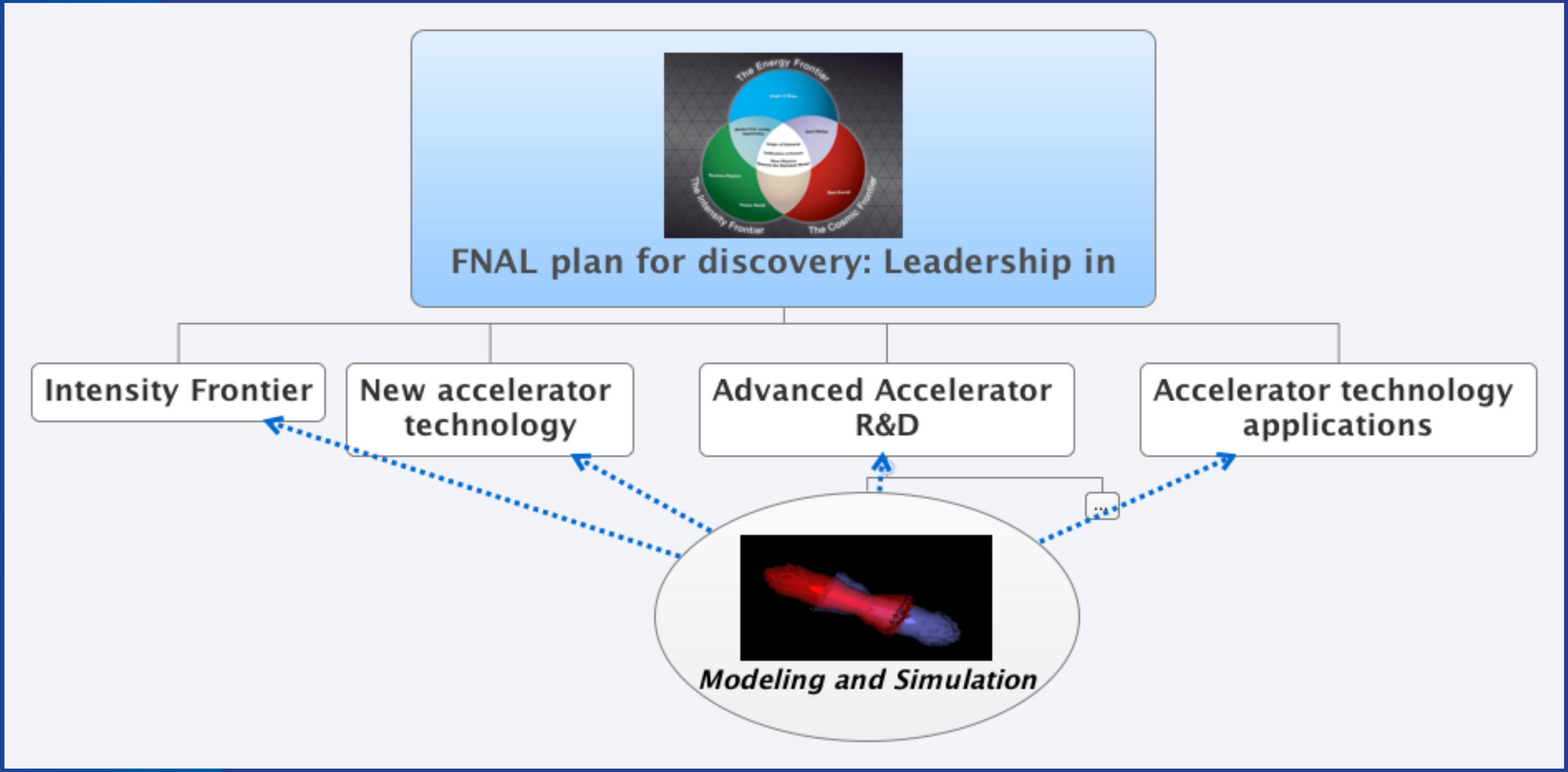
Numerical Simulation and Modeling



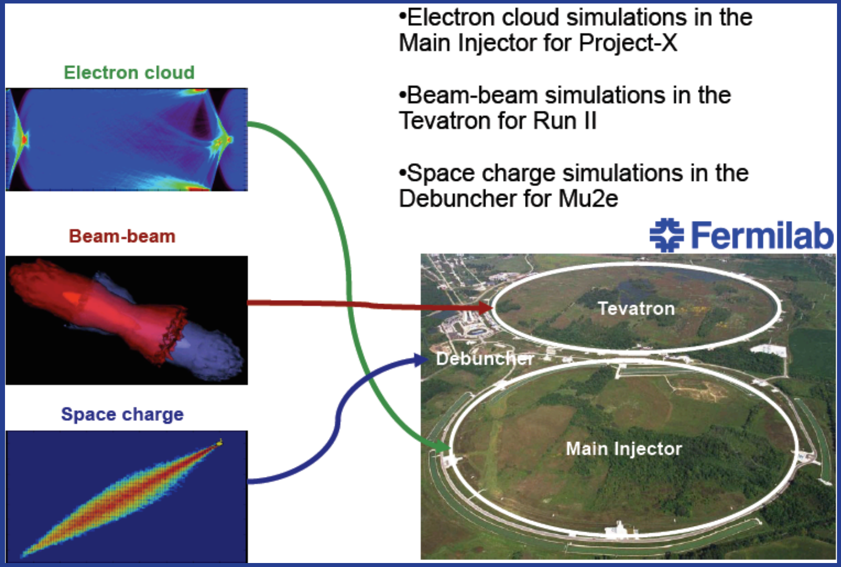
- Computational physics is an essential component of accelerator science, complementing and adding to experiment and theory
  - Goals are driven by the other strategic area needs, and the need to develop the necessary computational capabilities

Accelerator Simulation Development

- Computational infrastructure development requires significant investment; focus on tools and algorithms common to many applications
  - Of course, numerical methods are used in many different areas of Accelerator Science at FNAL, not all will be covered in this discussion
- Maintaining such capabilities is affected by evolving computing architectures
  - Models have to continuously be adapted and optimized
- Application development requires specialized expertise
  - Partnerships between application and computational scientists

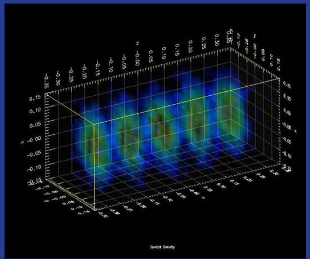
Computational Physics in Accelerator Science at FNAL

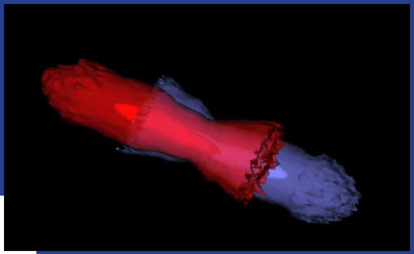
- A mature activity (more than 10 year involvement)
  - '96-'02 ionization cooling (μ-collider/ν–factory)
  - '01-'11 multi-particle dynamics (Run-II)
  - '01-'07 single and multi-particle, electromagnetics (ILC)
  - '09-... Single-particle, multi-particle (Project-X, Mu2e, …)
- Emphasis on
  - Advanced computational resource utilization
  - Realistic applications (multi-scale, multi-physics)
- Supporting and driving R&D

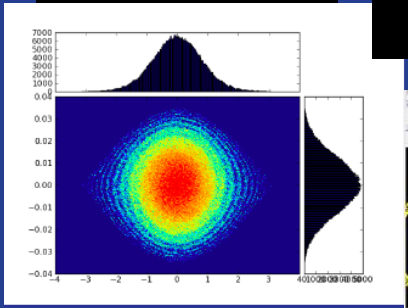


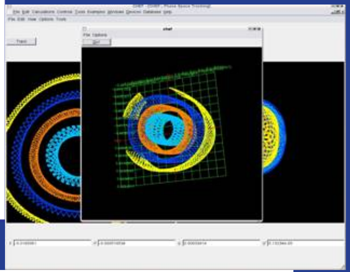
Major thrust areas of computationally challenging science

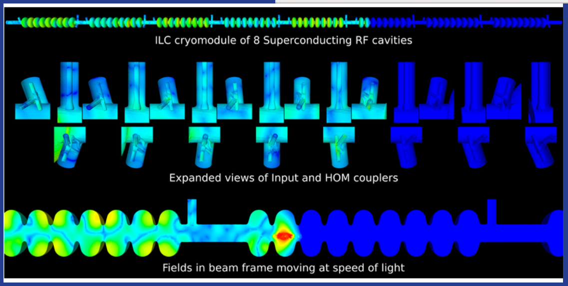
- Understand evolution of beams through optical systems, including self forces and the forces of interactions
  - Beam-beam, space-charge, electron cloud, …
  - Steering and phase-space manipulation systems (optics, cooling, …)
- Design of structures to maximize acceleration while minimizing deleterious effects of wakefields, heating, multipactoring, …
  - Electromagnetics, thermal, mechanical
- Advance accelerator science
  - Laser and plasma wakefields
  - Muon capture and acceleration

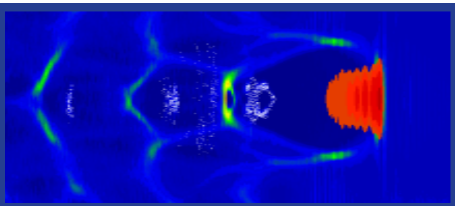












BTW, all models are wrong, some models are useful

Ultimate goal is to maximize the usefulness of our models

Long term goals for tools development

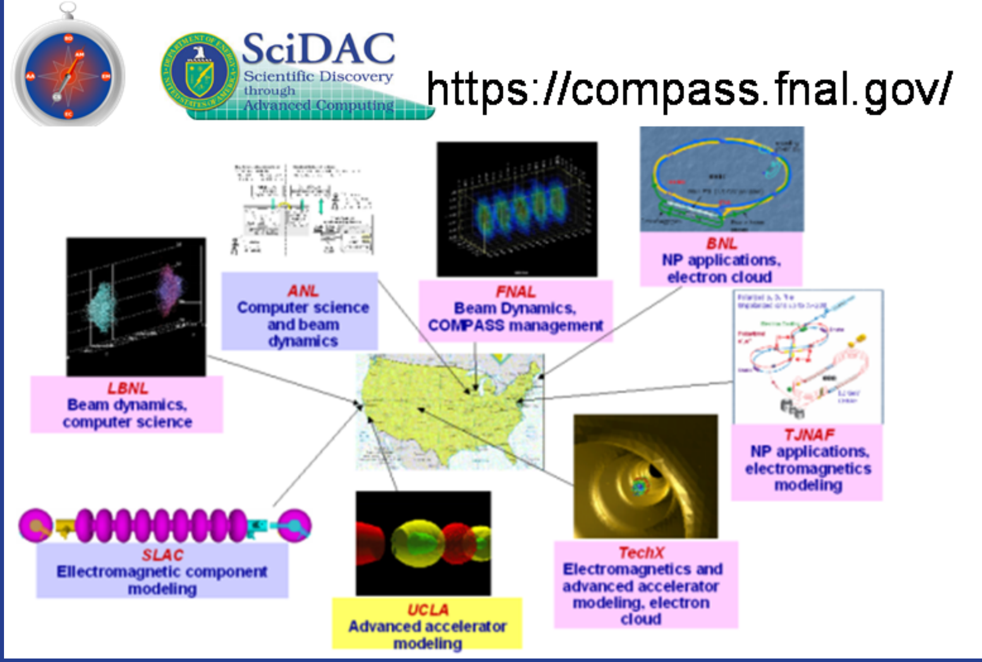
- Provide simulation support and guidance to future lepton collider design and R&D
  - Electron or muon, conventional or wakefield or ?
    - Develop expertise on required tools, develop and deploy required new capabilities
- Provide simulation support for parameter optimization of Project-X accelerators
  - in preparation for commissioning
  - design for possible interface with neutrino factory
- Deploy computational and physics algorithms that continue to take advantage of Leadership Computing Facility resources

How do we reach these goals: plans, issues

But first, where are we now

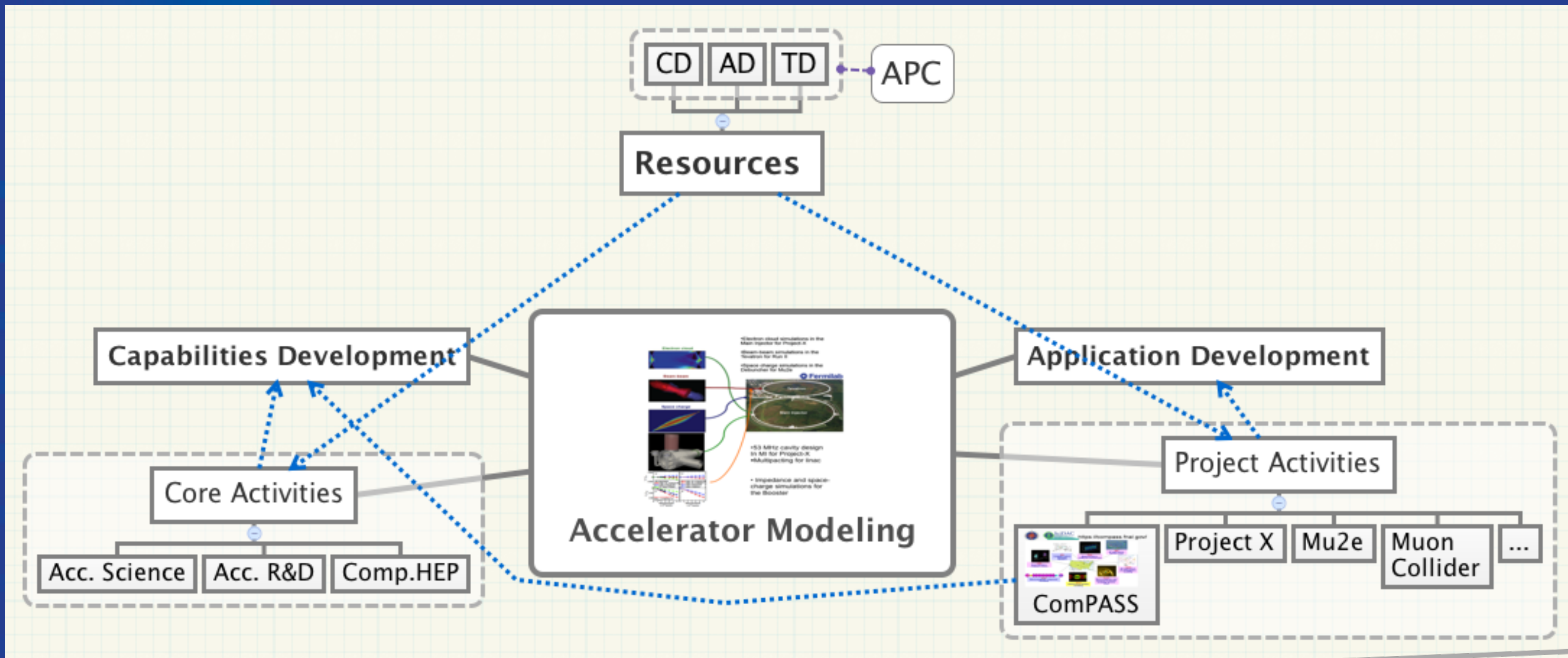
Accelerator Modeling Project: ComPASS*

- Fermilab leads the SciDAC2 ComPASS project, which aims to develop HPC accelerator modeling tools for
  - Beam dynamics: multi-physics, multi-scale
  - Component design: thermal, mechanical, electromagnetic
- Funded by the offices of HEP, ASCR, NP and BES at $3M/year
- The Fermilab team focuses on beam dynamics tools and application development

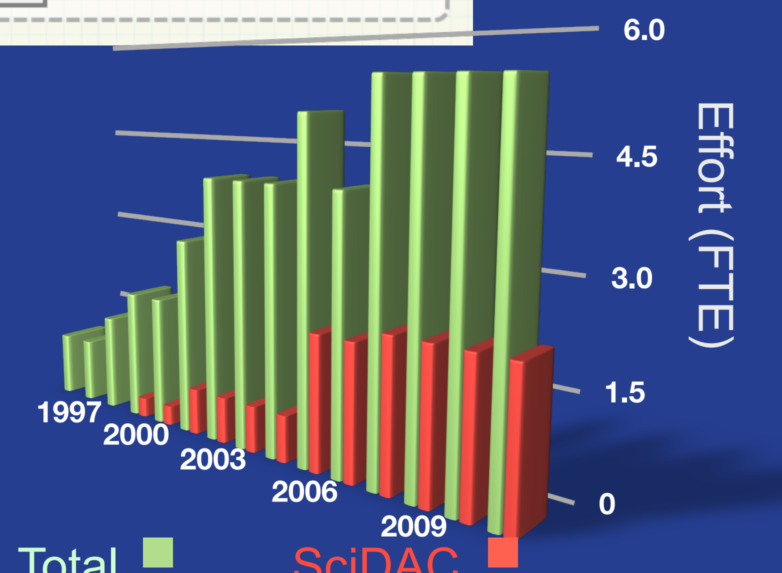


*Community Project for Accelerator Science and Simulations

Activities are highly leveraged

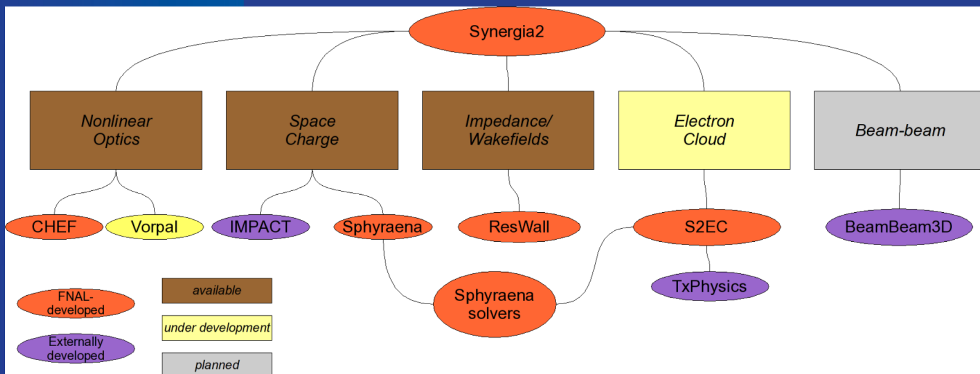


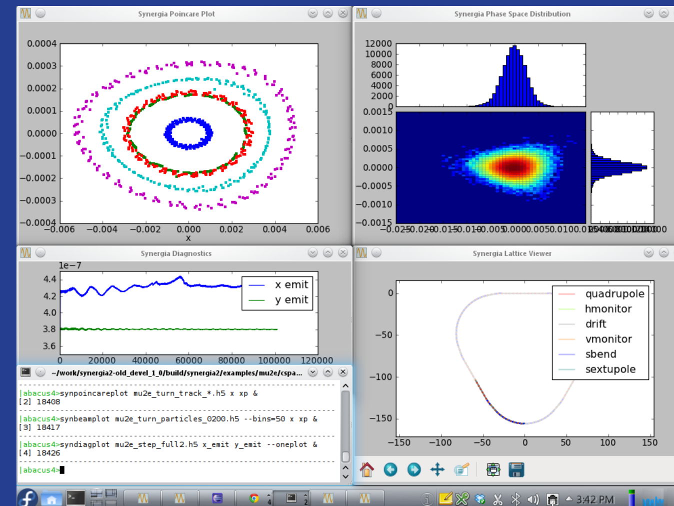
A well balanced but sensitive ecosystem!



- ComPASS & core supports computational capability development and provides access to
  - HPC resources
  - Math, computational and accelerator science expertise
- Projects support applications

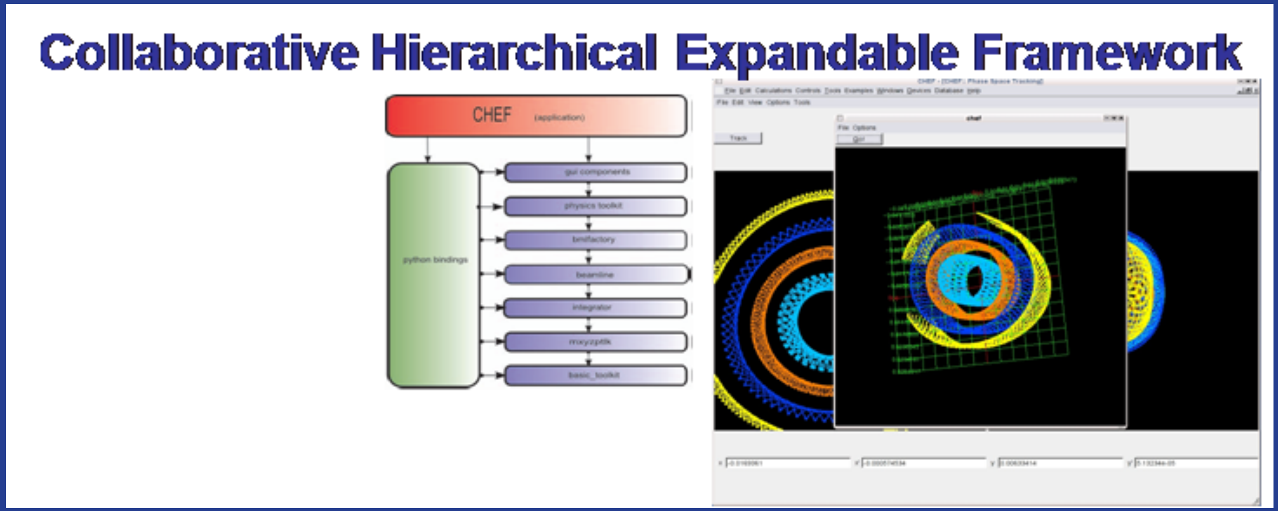
ComPASS tools development: Synergia





- Beam Dynamics framework with fully 3D PIC capabilities
  - Utilizes both native and external physics modules/algorithms
  - Includes space-charge & impedance (single and multi-bunch)
  - Single-particle physics from CHEF
- Runs on desktops, clusters and supercomputers
- Flexible framework allows for fully dynamic simulations including ramping, feedback, etc

Tools development, continued: CHEF



- CHEF originally developed at Fermilab starting in the early 90's
- Single-particle optics with full dynamics
- Can be reduced to arbitrary-order maps
  - We have done demonstration calculations in Synergia to 15th order
- Supports customizable propagators (fully extendable)
- MAD and XSIF parsers
  - Internal representation not limited by MAD parameters

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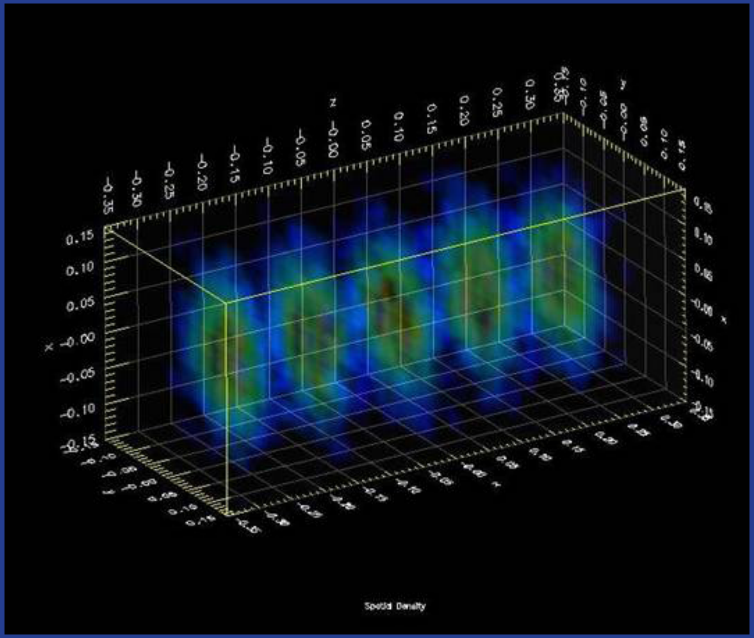
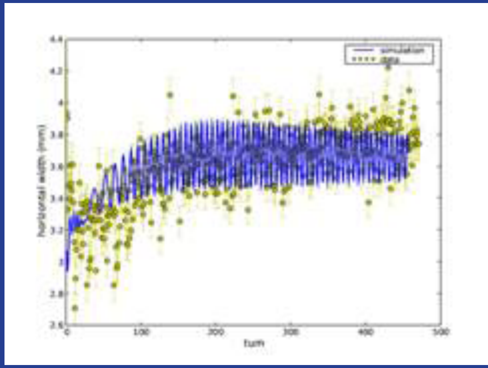
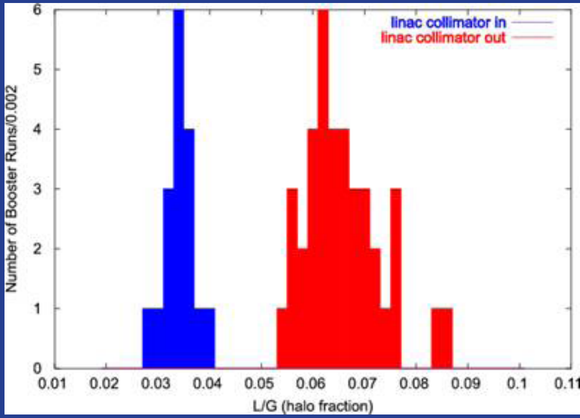
Space charge capabilities developed for Run II support

- Extensive modeling of the Booster with Synergia
  - 400 MHz structure debunching and 37.7 MHz capture
  - Including machine ramping
- Emittance growth and halo formation studies
  - Comparison with experiment
  - Used to help optimize operating parameters
    - Work with proton source department personnel
  - NIMA570:1-9,2007







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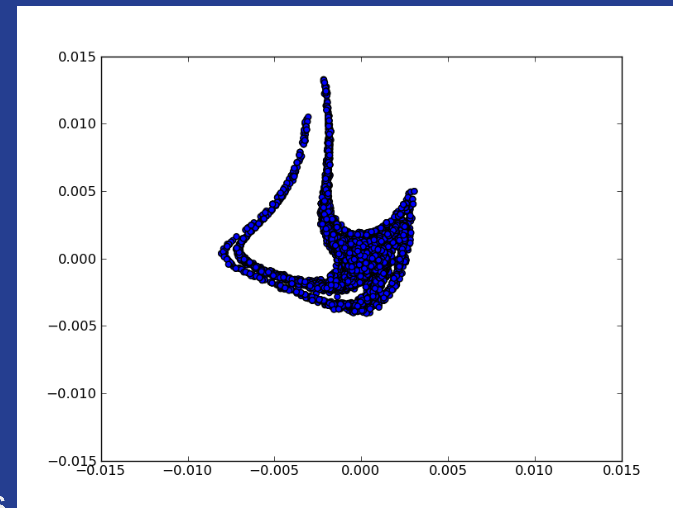
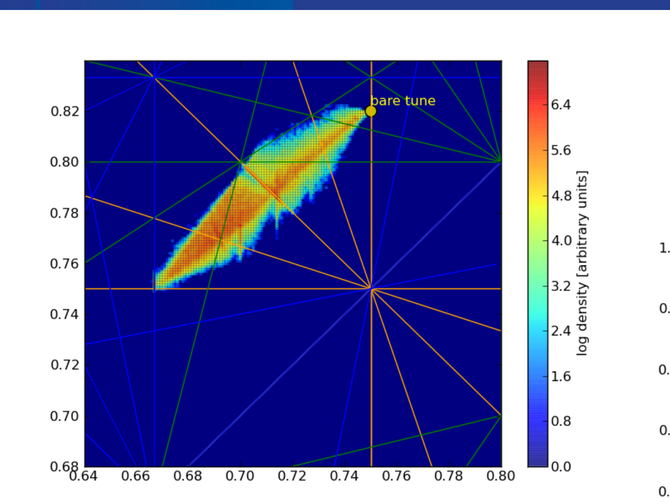
Current application: Mu2e extraction design

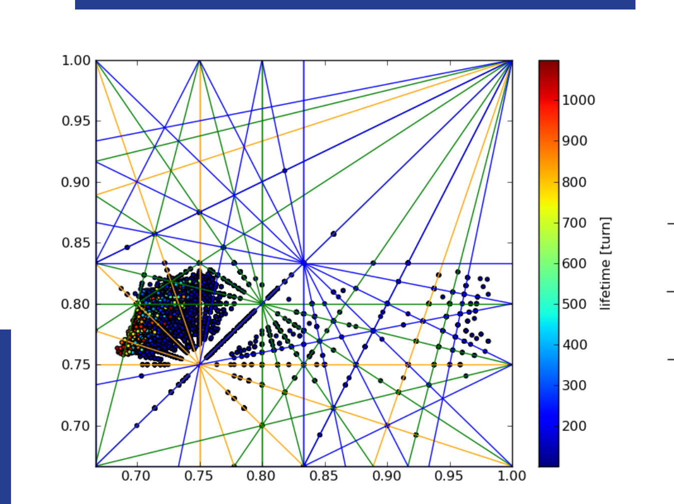
- Model resonant extraction including space-charge at the Debuncher :
  - Optimize tune and resonant extraction parameters to minimize losses

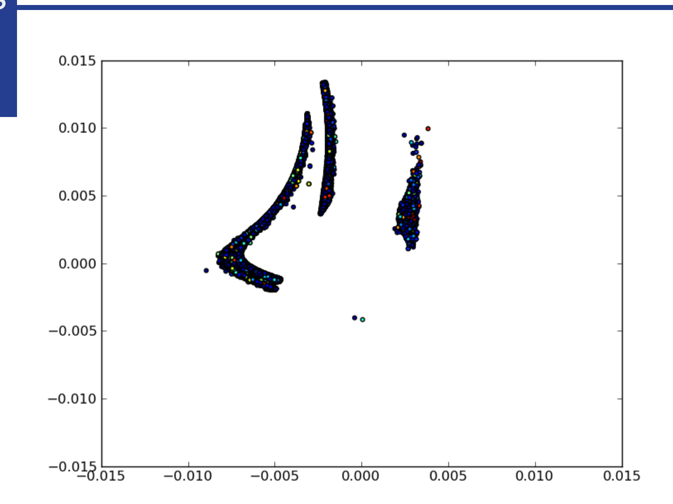


ν_x=9.75, ν_y=9.82

- phase space of entire beam
- phase space of lost particles
- tune footprint
- tunes of lost particles



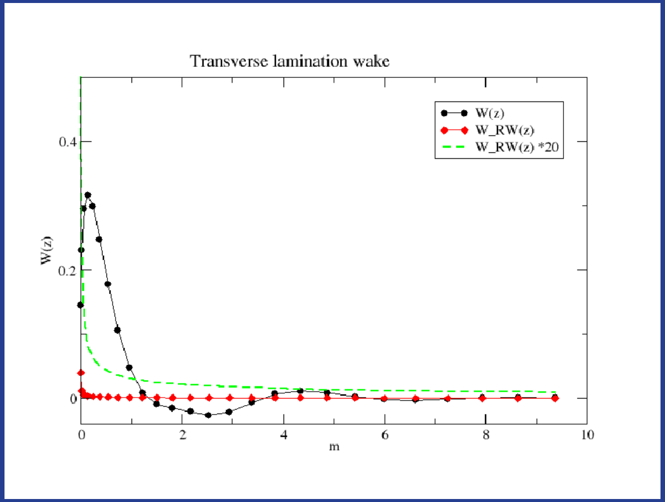


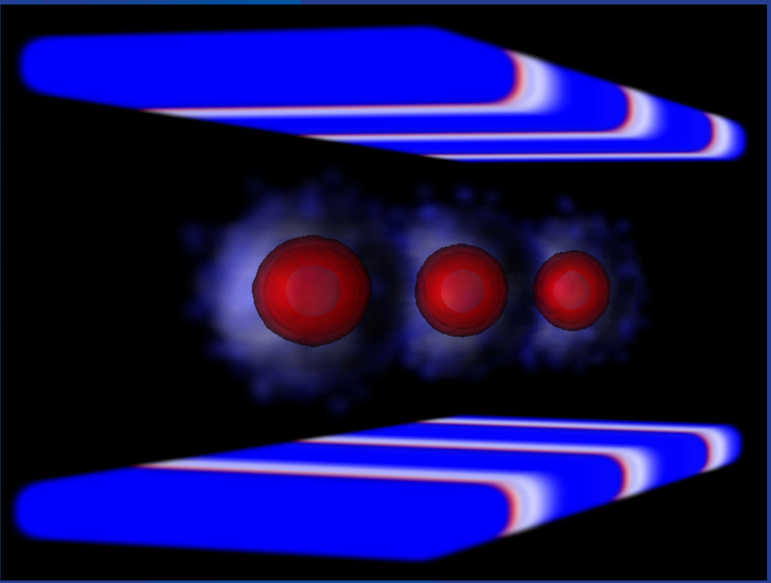


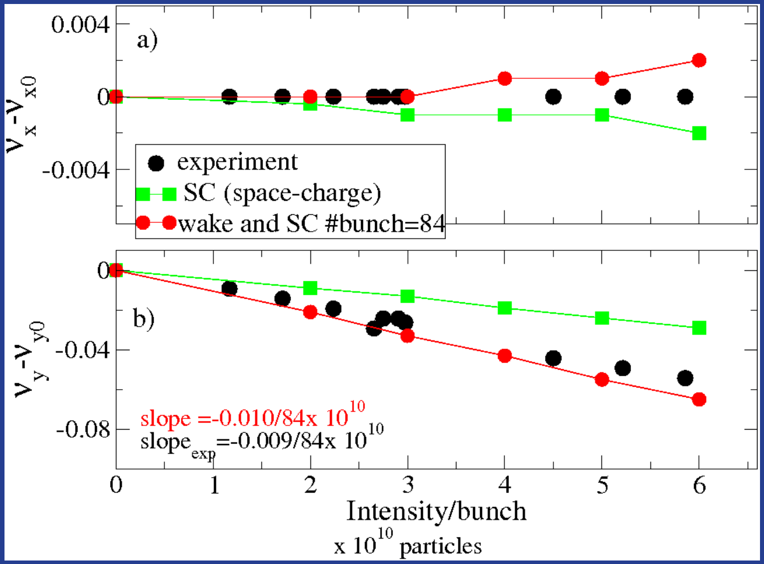
Continuing with Booster: careful treatment of impedance of laminated structures

Literature calculations in frequency domain involving different regimes don't trivially translate to a "simulation ready" wake function.

- Develop model, validate with FNAL Booster data, Phys.Rev.ST Accel. Beams 14:061003,2011
- Capability will be used for PIP support

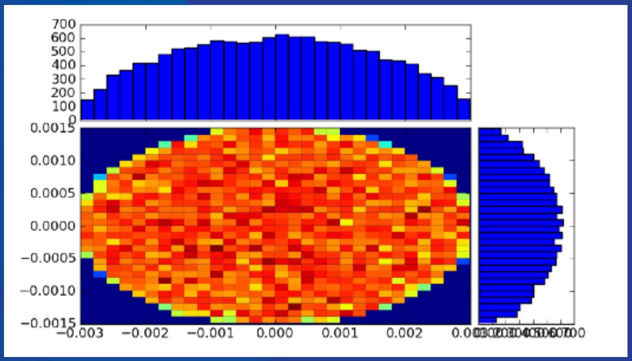


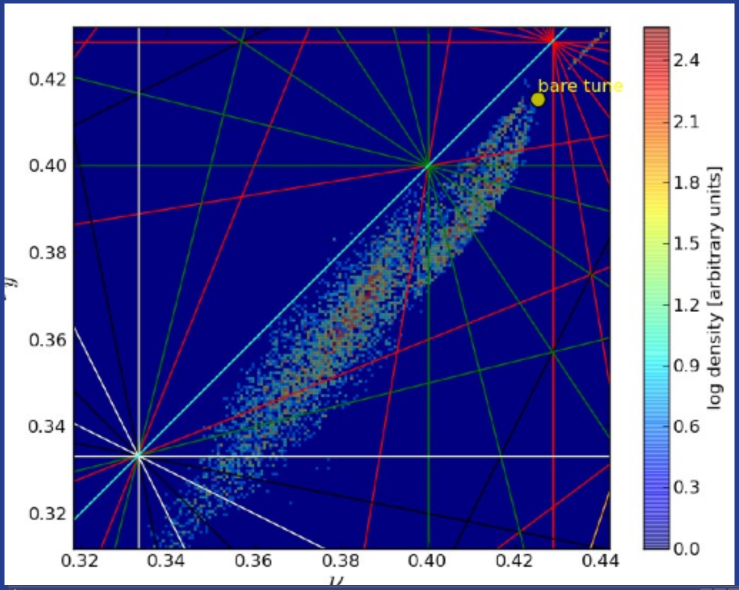


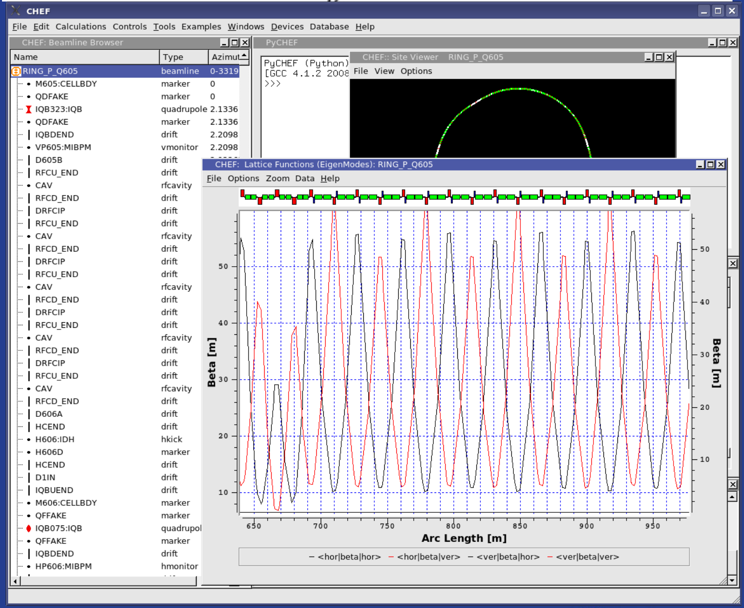


Current application : MI space-charge

- Begin modeling space charge effects and mitigation techniques for Main Injector with Project-X beam parameters
- Extend Synergia to include realistic apertures and fringe fields and study losses and mitigation, if necessary

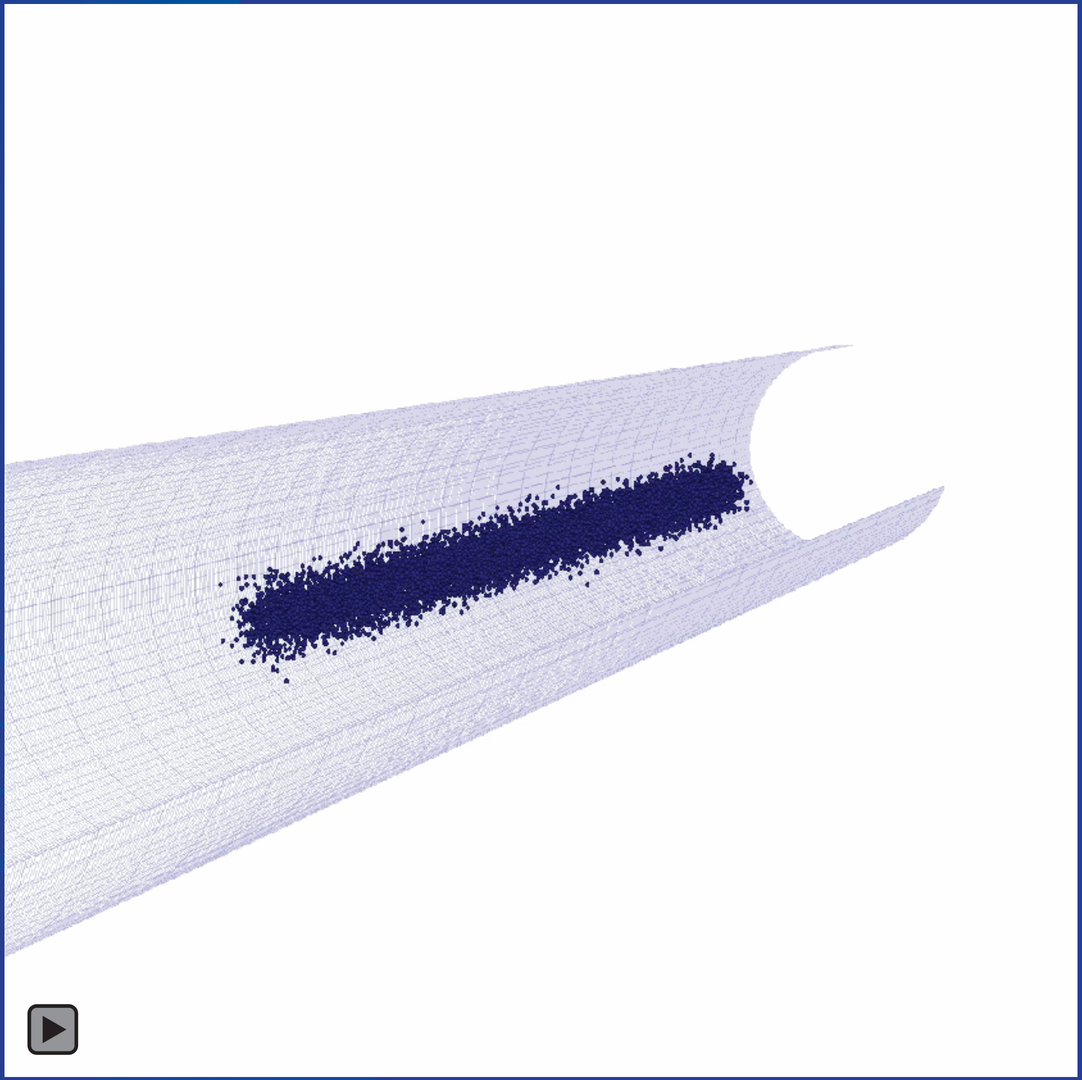




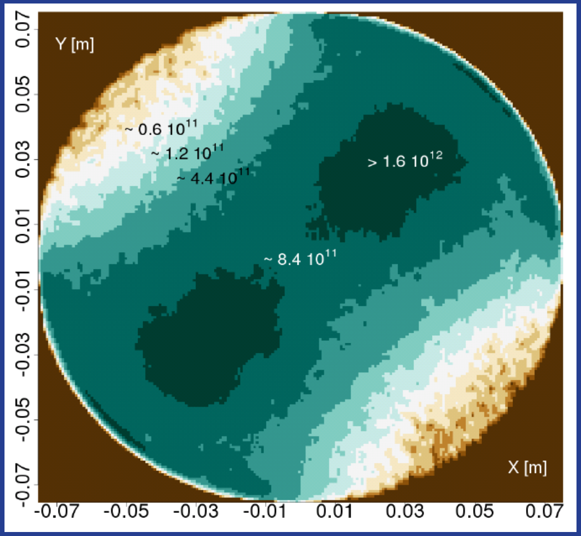


Utilization of ComPASS tools example

ComPASS VORPAL e-cloud simulation of MI experiments



Model microwave experiment (only possible with ComPASS tools), RFA response, code comparisons with “standard” tools such as POSINST



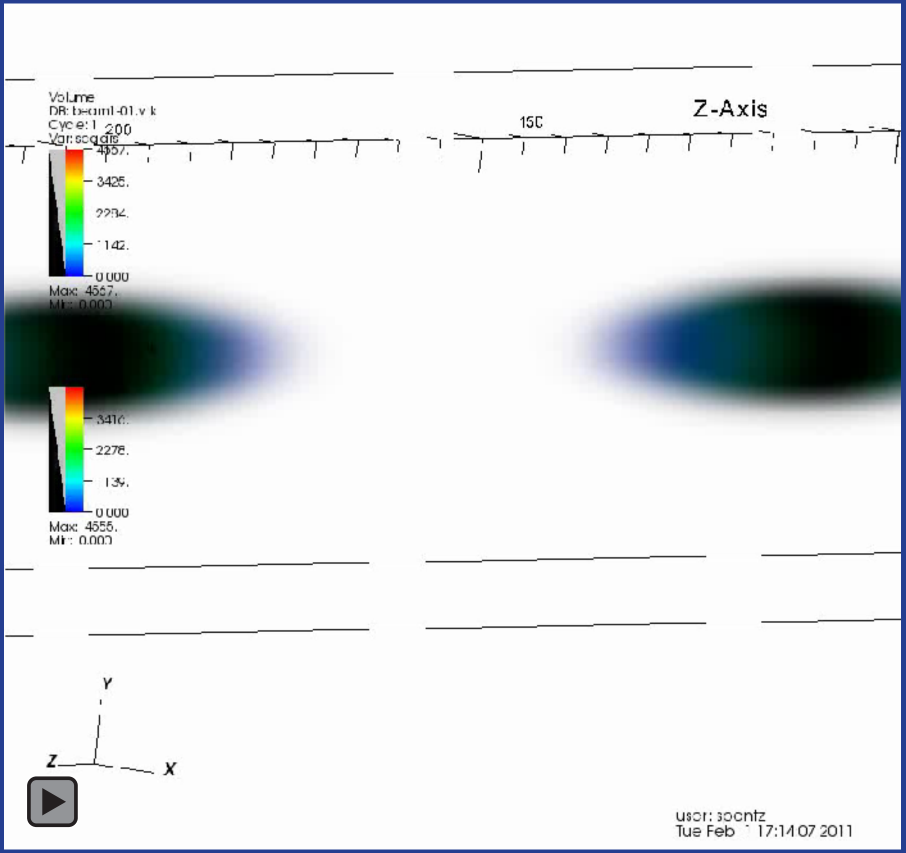
FERMILAB-PUB-11-228-APC-CD, submitted to PRSTAB

(A SciDAC Highlight) Tevatron example

- Improve Tevatron performance: understand beam-beam & impedance effects with 36 on 36 bunches
  - Simulations only possible with HPC resources: runs at NERSC and ALCF used 6M core-hours

- Success! Simulations result in improved operating parameters; reduce losses thus reducing radiation damage and increasing luminosity (physics reach)!

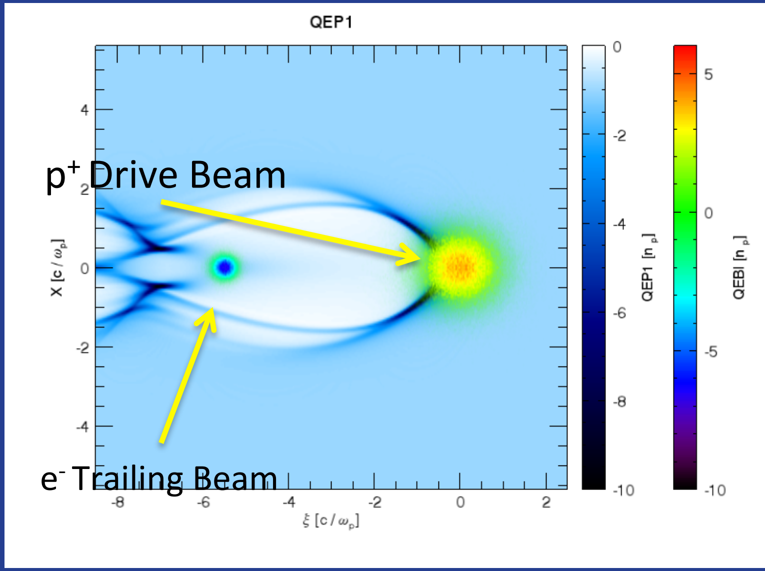
Phys. Rev. ST Accel. Beams 13, 024401 (2010)

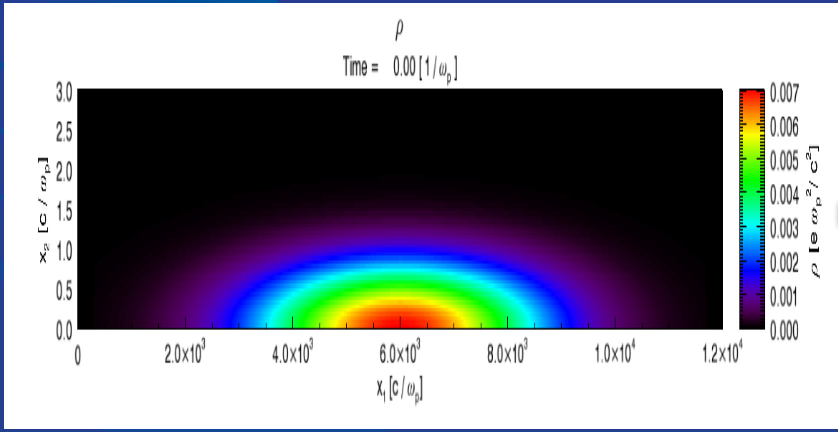


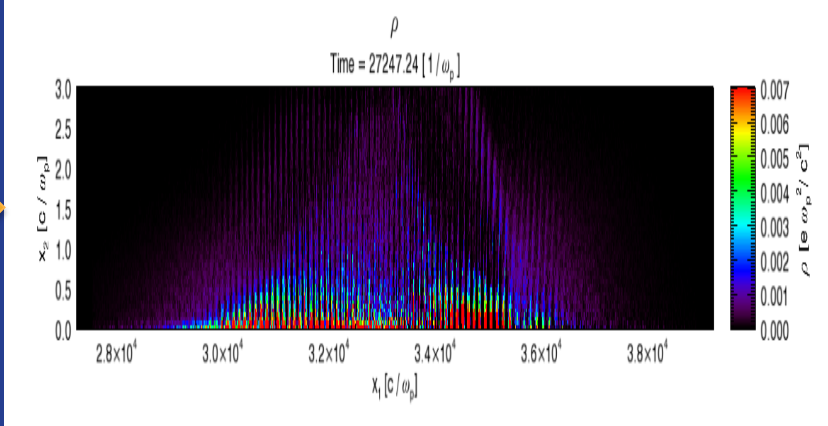
BeamBeam3D modeling of collective effects in Tevatron beam-beam collisions

Example of collaboration benefits: proton driven PWFA (protoplasma)

- Work with UCLA (W. An, C. Joshi, W. Mori) to explore possibility of a proton driven PWFA at FNAL (protoplasma, see Charles's talk)
- Utilize OSIRIS and QuickPIC, partially developed under COMPASS







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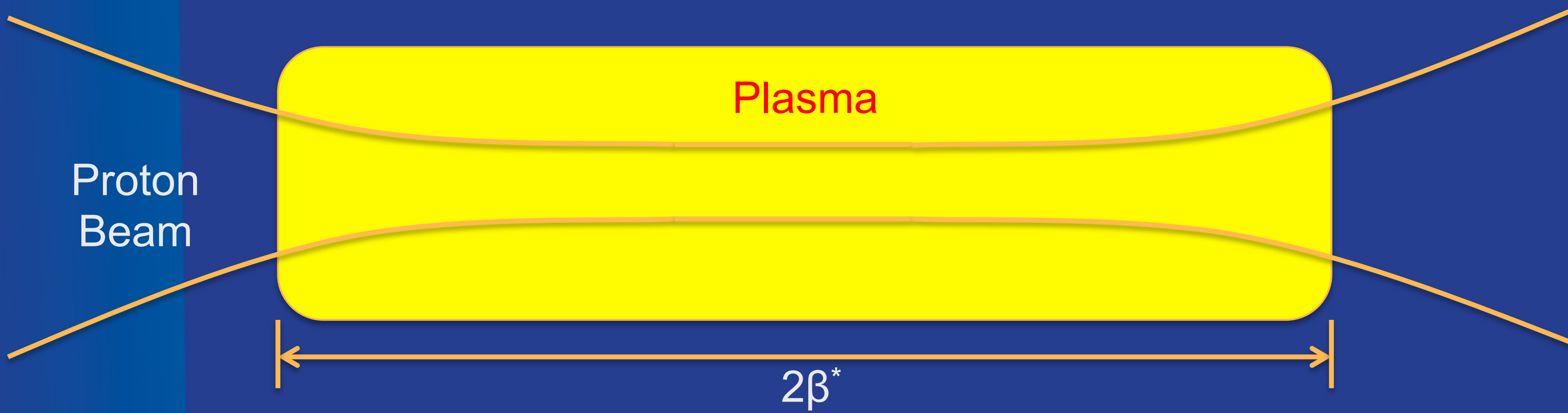
Support model for such activity

- We started exploring self-modulation parameter space for MI beam, at B0, using Tevatron final focus
  - Try to keep plasma cell “reasonable” (2m)
  - Study beam propagation in the plasma
- The tools need to be developed further to allow
  - Model injection, the beamline after the plasma, both for design and to understand tolerances, measurement issues
- Would like to explore feasibility of proof of principle experiment, using compressed Booster beam, without relying on self-modulation
  - PDPWA simulations are encouraging, but the experiment will need to be designed
- So far, simulations are done by Weiming An, a UCLA grad student on FACET (sorry Mark). This is the type of opportunistic activity that to be sustained would benefit from the ability to hire post-docs or support students.

Conditions for SM-PDPWA



We want : $L_{plasma} > 2\beta^* > L_{instability}$

- The instability growth rate is ~exp(G) and $G \sim \left(\frac{n_b m_e}{n_p m_p 2\gamma} k_p \xi (k_p s)^2 \right)^{1/3}$, where s is the beam propagation distance in the plasma.

- Let this distance s = $2\beta^*$, then $G \sim \left(2 \frac{n_b}{n_p \cdot c} k_p \sigma_z \right)^{1/3}$, where $c = \frac{\sigma_{rM}^4}{2\sigma_r^4}$ is a normalized parameter and σ_{rM} is the matched spot size of the beam propagating in an ion column.

- Simulations indicate G needs to be large (> 10).

Parameter scan for SM-PDPWA

	n_p (10^{15} cm^{-3})	N (10^{11})	n_b/n_p (10^{-3})	ε_N (mm mrad)	γ	σ_r (μm)	σ_z (cm)	β^* (cm)	c (10^{-3})	G	L_{plasma} (cm)
Set 2	10	1	0.635	3.33	128.9	100	10	38.71	4.5	8.1	~200
Set 4	1	1	0.9	3.33	128.9	265	10	271.8	0.9	10.6	~500
Set 5	10	1	0.09	3.33	128.9	265	10	271.8	0.09	16.4	~500
Set 6	10	1	0.635	1.67	128.9	100	10	77.42	1.13	12.8	~200
SPS CERN*	0.7	1.15	2.17	3.845	480.6	200	12	500	1.4	12.3	~1000

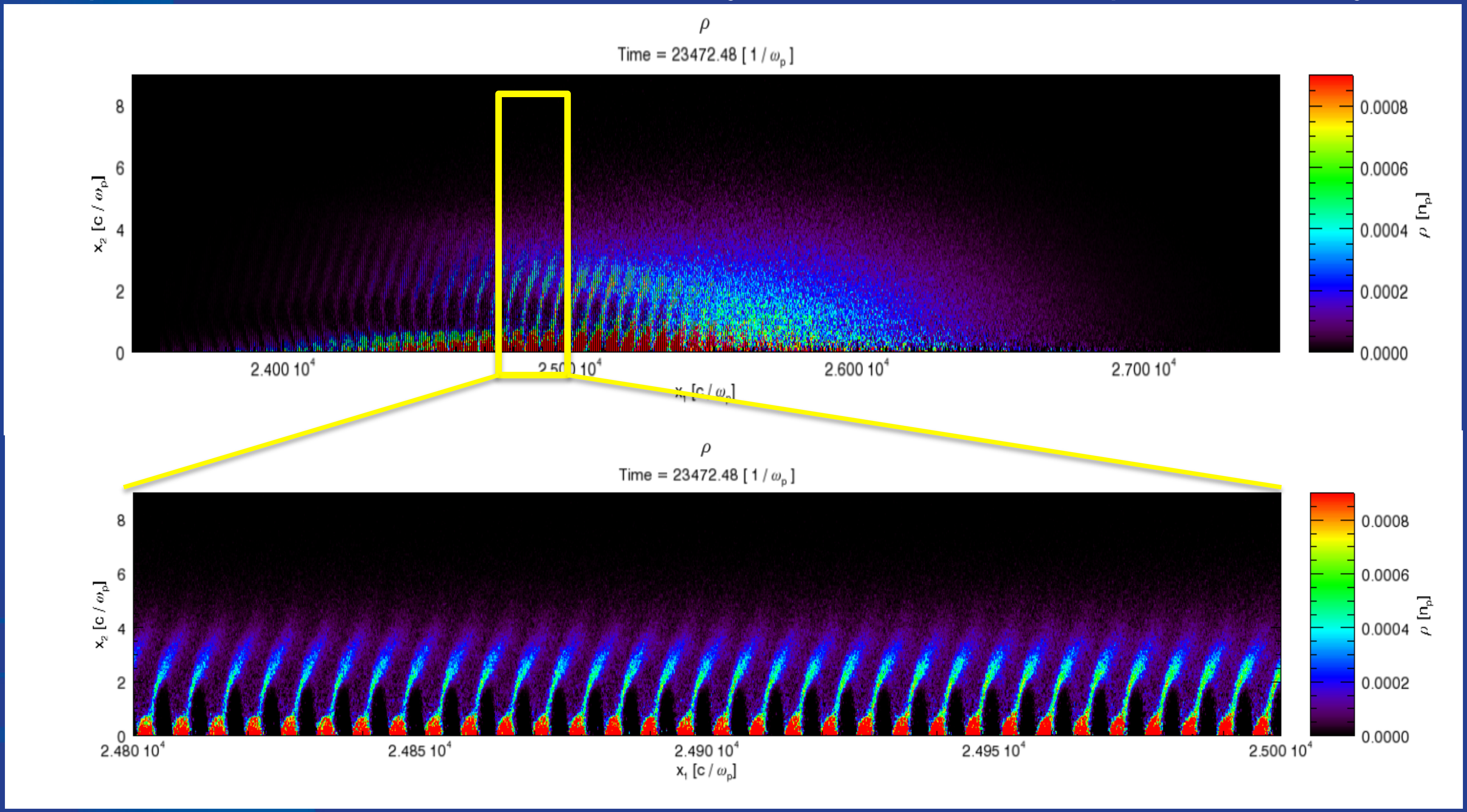
\+ Beam parameters are r.m.s. values.

In the OSIRIS simulations the beams are focused to the plasma entrance. To "emulate" a beam focused at β* inside the plasma we reduced the emittance by 2 (in Set 6). The code has to be extended to properly model parameters for short plasma cells (where we need to focus in the column).

* A. Caldwell, K. V. Lotov, Phys. Plasmas 18, 103101 (2011).

OSIRIS results of SM-PDPWA (Set 4)

Snapshot of the beam charge density at the time when the beam center propagating in the plasma for 290 cm. The beam density is normalized to the plasma density.



Beam Parameters (Set4): $N = 1 \times 10^{11}$, $\sigma_r = 265\ \mu m$, $\sigma_z = 10$ cm, $\varepsilon_N = 3.33$ mm mrad. Plasma Denstiy: $n_p = 1 \times 10^{15}\ cm^{-3}$

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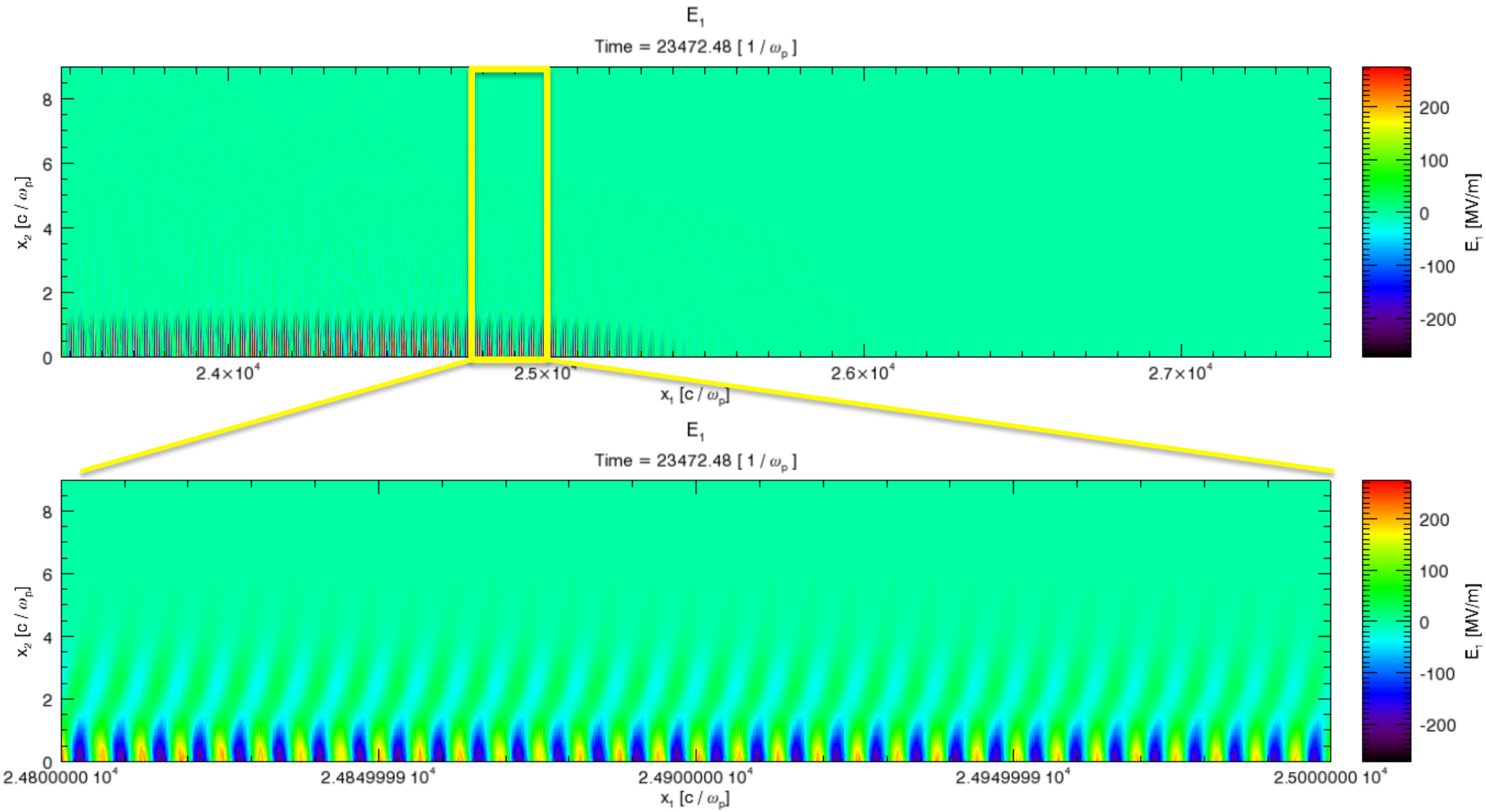
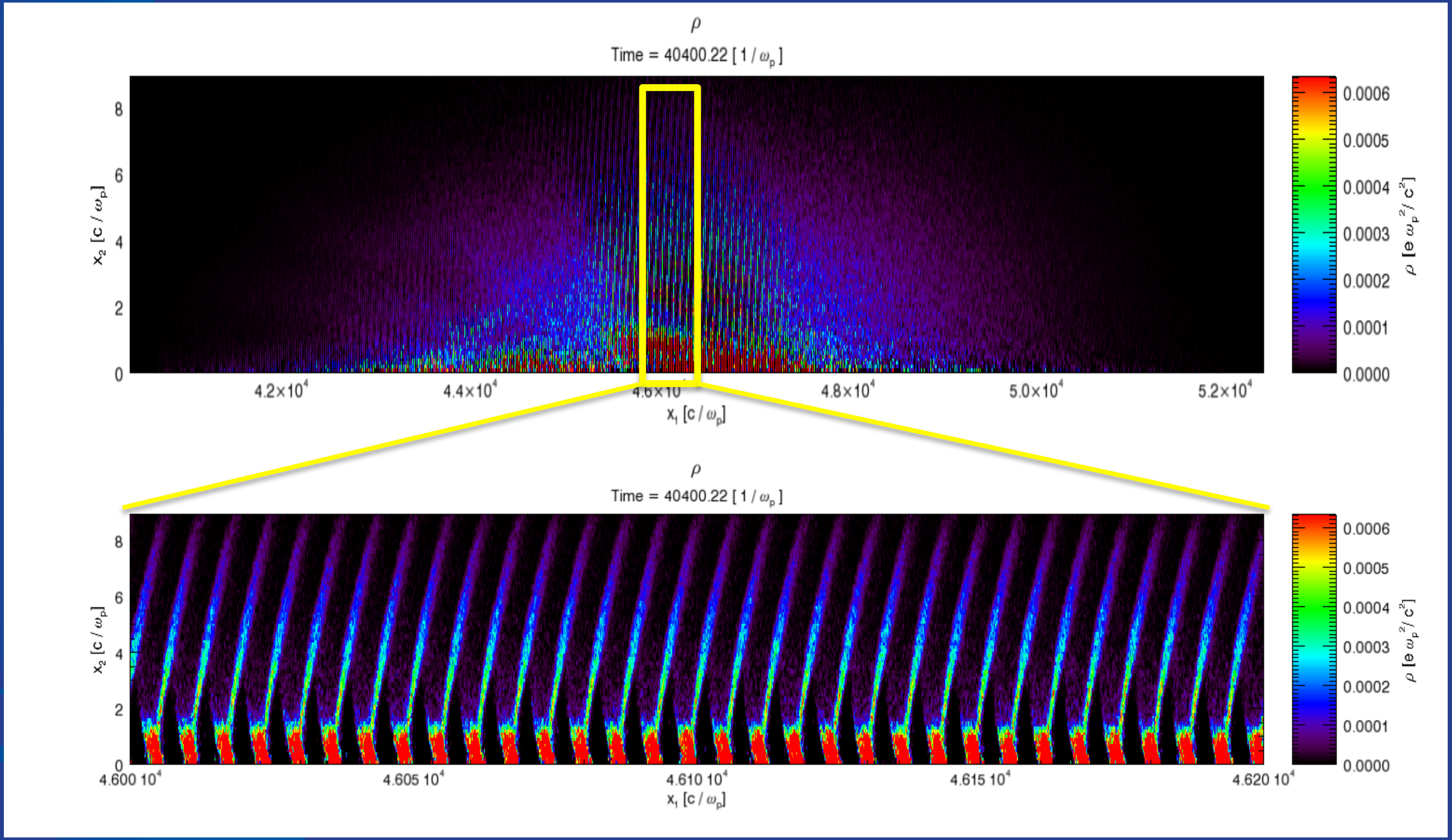
OSIRIS results of SM-PDPWA (Set 4)

Snapshot of the E_z at the time when the beam center propagating in the plasma for 290 cm. The maximum E_z reaches 270 MV/m at this time.



OSIRIS results of SM-PDPWA (Set 6)

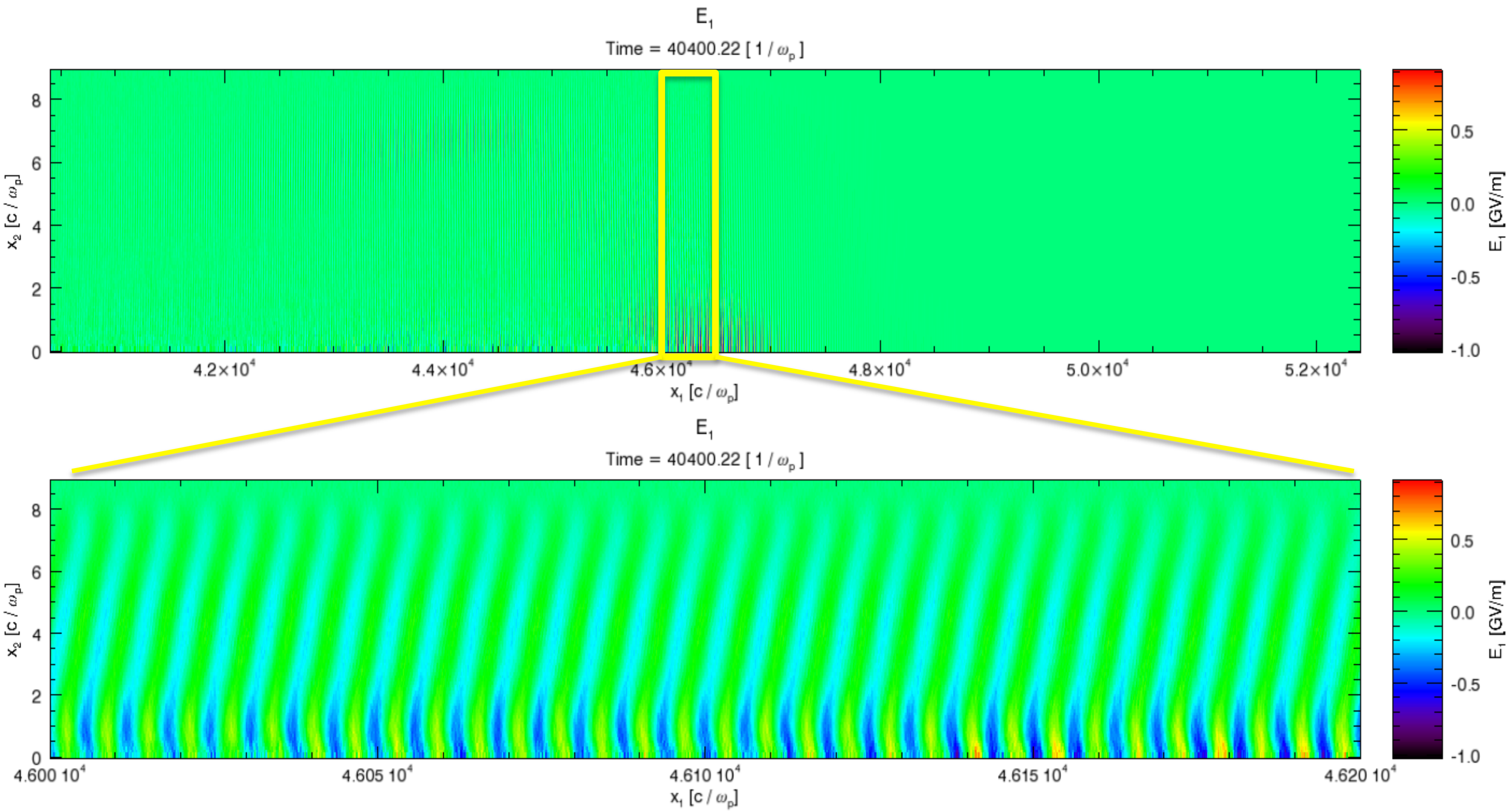
Snapshot of the beam charge density at the time when the beam center propagating in the plasma for 120 cm. The beam density is normalized to the plasma density.



Beam Parameters (Set6): $N = 1 \times 10^{11}$, $\sigma_r = 100\ \mu m$, $\sigma_z = 10$ cm, $\varepsilon_N = 1.67$ mm mrad. Plasma Denstiy: $n_p = 1 \times 10^{16}\ cm^{-3}$

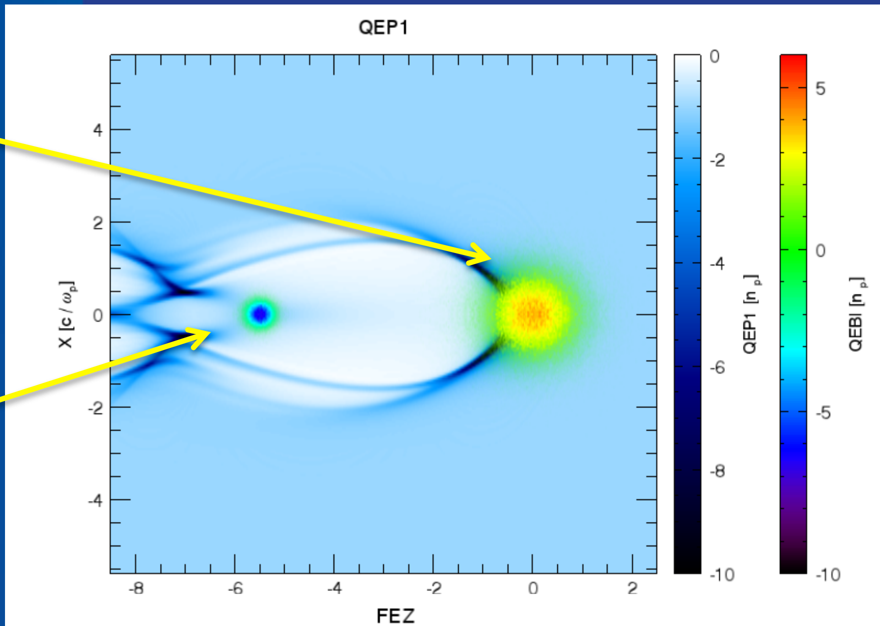
OSIRIS results of SM-PDPWA (Set 6)

Snapshot of the E_z at the time when the beam center propagating in the plasma for 120 cm. The maximum E_z reaches 1 GV/m at this time.



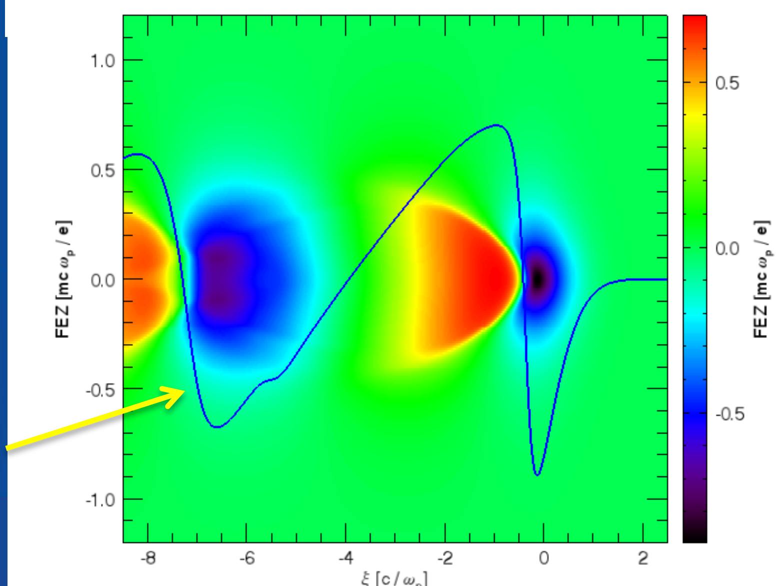
Plasma Wake Field Driven By A Compressed 8 GeV Proton Beam

p^+ Drive Beam



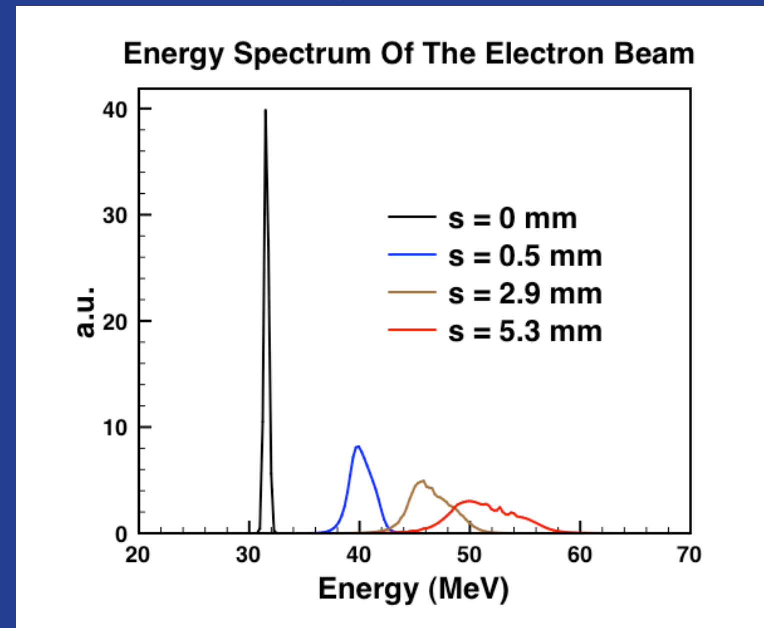
e^- Trailing Beam

Field flattened due to beam loading.



Beam Parameters: E = 8 GeV, N = 0.6 x 10^{11}, σ_r = 100 μm, σ_z = 100 μm, ε_N = 3.33 mm mrad

Plasma Denstiy: $n_p = 1 \times 10^{15}$ cm^{-3}



This preliminary simulation shows that the trailing electron beam can obtain 20 MeV energy gain within 5.3 mm propagation in a 10^{15} cm^{-3} plasma. The energy gain is limited by the dephasing.

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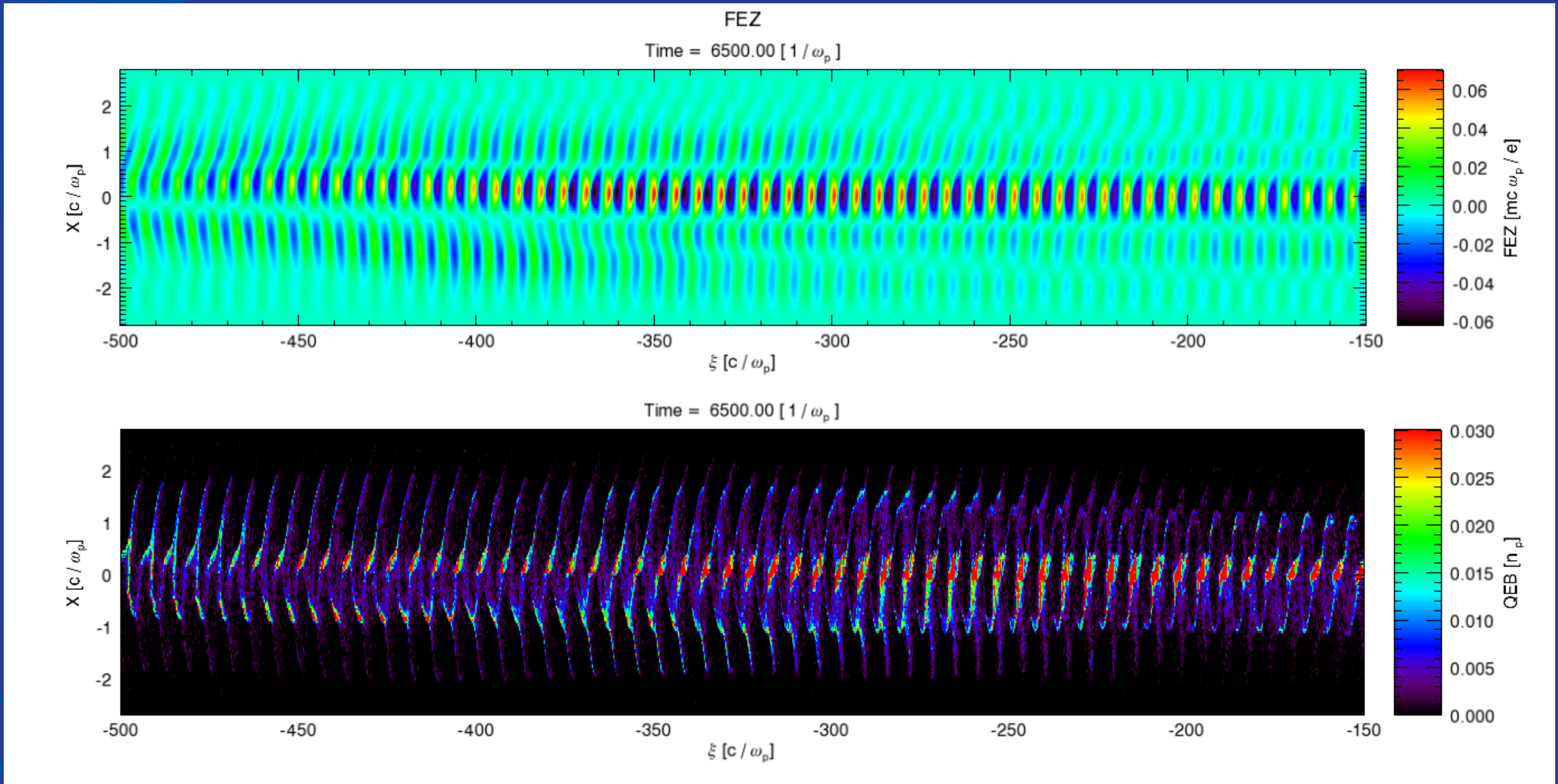
3D Effects Of SM-PDPWA

QuickPIC simulation results show that 3D effects may be important. We can find that the proton beam is deflected in a self-modulated regime. More investigation is needed (including studying ion mobility effects).



Partially Enlarged E_z and beam density plot after 35 cm propagation in the plasma. The plot is a 2D slice from a 3D data along the transverse direction x (at y = 0).

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Computing is evolving: new architectures

- What will they look like?
- GPUs, SIMDs
  - How to move forward: porting code and developing new code
    - ➢ Parallel scalability

SIMD units

VMX SSE/2/3/4

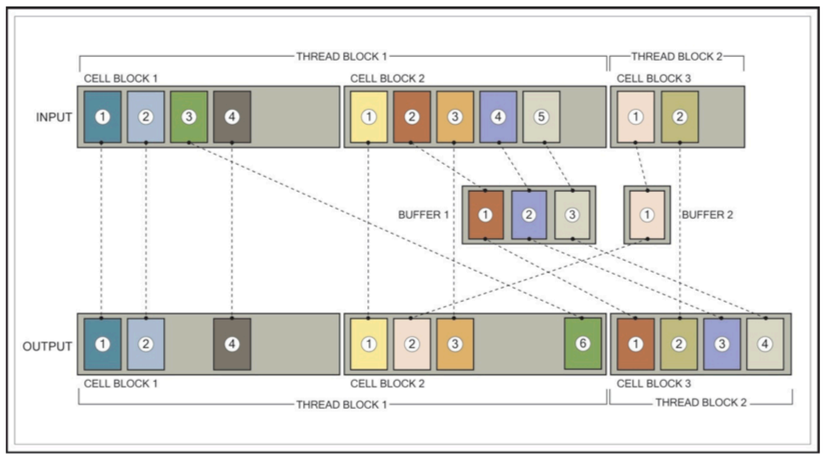
GPGPUs

CUDA STREAM

- SIMD
  - Vector co-processor
  - Available in most common CPUs
- GPGPU
  - Graphics Processing Units
  - Up to ~ 1 TFlop/s per board
  - “Add-on” co-processor
- Ultra-Massively Parallel
  - Scalability to over 10^5 cores

R&D: GPU acceleration for EM PIC

Solver Step	Intel Nehalem (ns)	Tesla C1060 (ns)	Fermi C2050 (ns)
Push	81.7	1.13	0.89
Deposit	40.7	1.06	0.78
Sort	0.5	1.13	0.57
Total	122.9	3.32	2.24

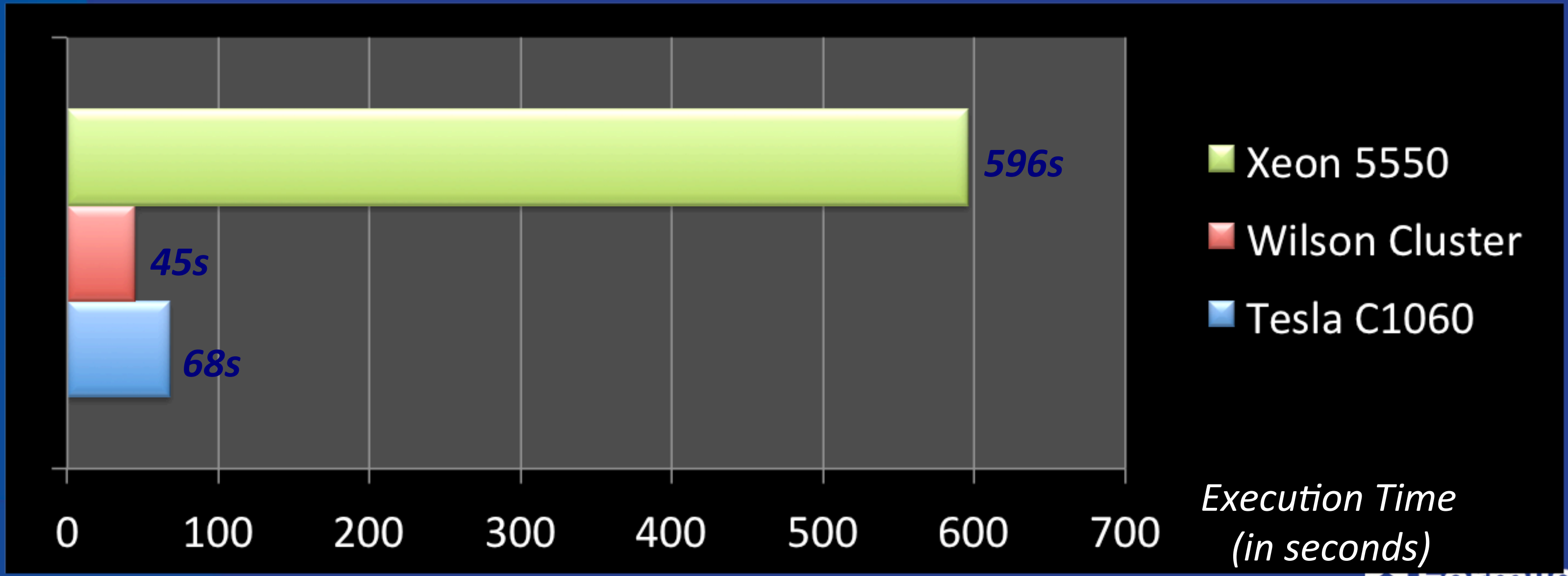


- Algorithms are hybrids of previously used techniques
  - Vector (from Cray), tiling (from cache-based), domain decomposition with particle re-ordering (from distributed memory)
- Overall speedup of about 55 for 2+1/2D EM PIC code

➢ **This is a new activity for ComPASS, in-house effort, we will need to formalize and define within SciDAC3 and co-design center era!**

R&D: GPU acceleration for electrostatic PIC

- Benchmark Problem:
  - Grid of 64x64x512 = 2,097,152 cells, with 20,971,520 particles (10 particles per cell)
- Comparison systems:
  - **1. Intel Xeon X5550, single process @ 2.67GHz;**
  - **2. Fermilab Wilson Cluster, dual Xeon X5650 2.67GHz nodes with 10Gbps Infiniband interfaces. 16 nodes / 128 cores used**
  - **3. NVidia Tesla C1060, 30 streaming multi-processors @ 1.30GHz in a single GPU**



Risks and opportunities

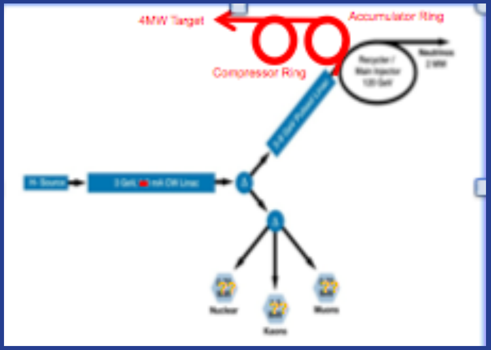
NEAR-TERM ACTIVITIES

Capability Development

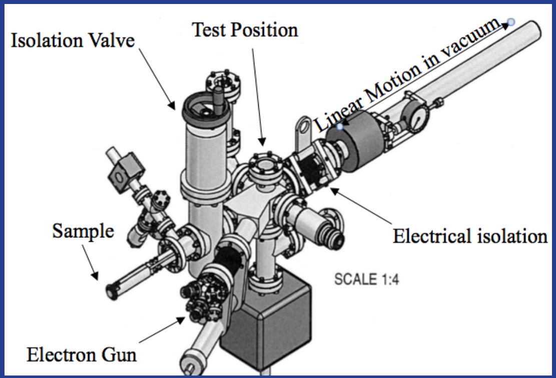
- Deploy parallel optimization algorithm (a ComPASS deliverable, currently under development)
  - Multi-parameter optimization needed by most applications.
- Electron cloud capability improvements
  - Incorporate new experimental data
  - Models for (almost) self-consistent cloud+beam dynamics
    - Consider dielectric plasma representation of cloud
- Incorporate plasma code capabilities in beam-dynamics frameworks (a ComPASS goal for collider design)
  - FNAL goal: protoplasma
- Continue R&D on algorithms for new computing architectures
- Continue performance optimization of current algorithms
- ComPASS funding cycle ends in FY12. New proposal due first quarter of FY12
  - If not extended, reduced support for capability development, loss of access to non-FNAL HPC capable codes and expertise

Program Support

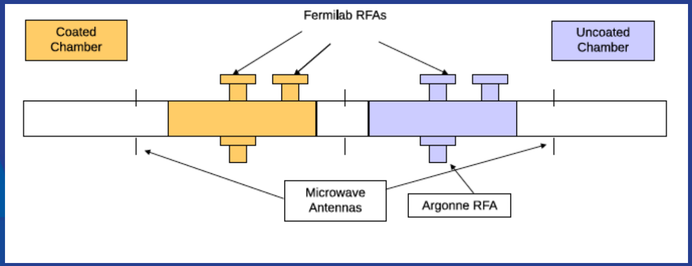
- Opportunity: Muon collider design, especially interface with P-X driver
  - Will benefit from parallel optimizer
  - Need to establish better collaboration with MAP



- Opportunity: Protoplasma experiment design
  - Requires integration of plasma and conventional beam dynamics tools
  - R&D effort needs to be seeded (postdocs)



- Continue to support e-cloud experimental program

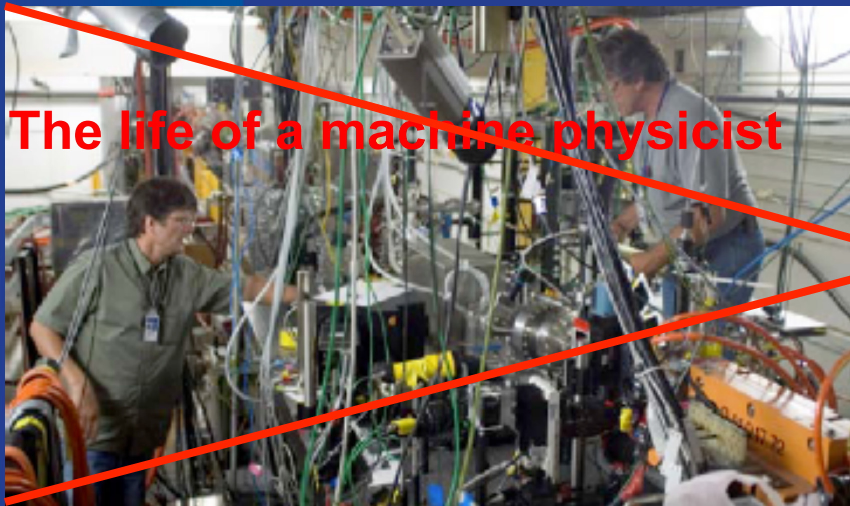


Program Support

- Continue studying space-charge effects in MI for Project-X era parameters
  - Study losses with realistic apertures and measured magnetic fields
- Provide simulation support for the PIP
  - Booster modeling of instability studies
- Continue Mu2e extraction design support
  - Implement RFKO (spill rate control) in model
  - Participate and support beam studies
- In general, all applications will benefit from improved code performance on HP machines and parallel optimizer deployment

Fermilab

Conclusions



- Computational accelerator physics must balance capability development R&D with accelerator science R&D support
- Work closely with machine physicists to maximize usefulness of numerical simulation utilization
- Leveraging resources essential, seeding new R&D efforts necessary for success